EXAFS Studies of Nanoscale and Nanostructured Materials Workshop

May 20, 2003

Motivated by the recent excitement of scientists in the field of nanoscience, which is the study of materials at a scale of a few billionths of a meter, physicist Vincent Harris of the Naval Research Laboratory (NRL) in Washington, DC, organized a workshop titled: "Extended X-ray Absorption Fine Structure (EXAFS) Studies of Nanoscale and Nanostructured Materials."

Although the workshop was tightly focused on the use of EXAFS to probe the nanostructure of materials, international speakers also covered magnetism, biology, geochemistry, catalysis, and electronics.

Physicist Scott Calvin, of NRL, chemist Josef Hormes, the director of the Center for Advanced Microstructures and Devices (CAMD), a synchrotron radiation research center at Louisiana State University in Baton Rouge, and chemist Robert Schloegl, of Fritz-Haber-Institute in Berlin, Germany, addressed the difficulties of quantitatively describing freestanding nanoparticles.

Physicist Anatoly Frenkel, of Yeshiva University in New York, made a presentation on nanoparticles embedded within a common amorphous host. Physicist Maria Grazia Proietti, of the University of Zaragoza in Spain, and environmental scientist Ken Kemner, of Argonne National Laboratory, presented their progress in the study of semiconductor quantum wires and nanoparticles formed via biogeochemical interactions, respectively.

Calvin and Hormes both presented talks focused on the use of EXAFS, specifically the use of FEFF-generated theoretical data together with FEFFIT fitting codes, to describe the local element-specific structure of nanoparticles and core shell nanoparticles. FEFF is a computer program created at the University of Washington that generates x-ray absorption fine structure spectra for clusters of atoms. This data is used by another computer program called FEFFIT to allow rapid fitting of unknown atomic structures.

Calvin's work includes the multi-edge fitting of mixed spinel ferrites and the passivation of metallic iron in multi-shelled nanoparticles. Calvin is particularly interested in the stabilization of high magnetic moment particles for applications ranging from high frequency electronics to magnetic targeted drug delivery. He described his nanoparticles as having multiple layers of amorphous metal and oxide surrounding a close packed Fe core.

In contrast, Hormes relied heavily upon XANES spectra to establish that the local structure of nanoparticles are indeed quite different from their bulk counterparts and that XANES spectra can be used to track the evolution of valency as the particle

Workshop Participants

size is increased during processing.

Schloegl presented a review of his work in the use of *in-situ* time resolved EXAFS to understand the local structure fingerprinting of the phase transformations of molybdates; a class of materials that hold potential for catalytic applications.

Proietti described the use of Grazing Incidence Diffraction Anomalous Fine Structure (GI-DAFS) to reveal the role of phosphorous in InAs/InP self assembled quantum wires. This talk was a balance of high quality semiconductor materials processing and extremely difficult techniques that left the audience thoroughly impressed.

Finally, Kemner showed the value of the APS as a state-of-the-technology synchrotron capable of probing the dynamics of ground water contamination in the burgeoning field of biogeochemistry.

Each speaker generated excitement and active question-and-answer periods that often spilled out into the corridors. Materials scientist Joseph Woicik, of the National Institute of Standards and Technology (NIST) reminded the attendees of the value and importance of presenting raw data for inspection by the audience.

In summary, the key findings of the workshop were that EXAFS is a near-ideal tool for the characterization of nanoscale systems, but that it is best used with other techniques to provide scientists with a clearer picture of the material under study.

-Vincent Harris